

09831954

FILE 'HOME' ENTERED AT 14:21:22 ON 14 NOV 2002

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:21:32 ON 14 NOV 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 NOV 2002 HIGHEST RN 473527-47-8

DICTIONARY FILE UPDATES: 13 NOV 2002 HIGHEST RN 473527-47-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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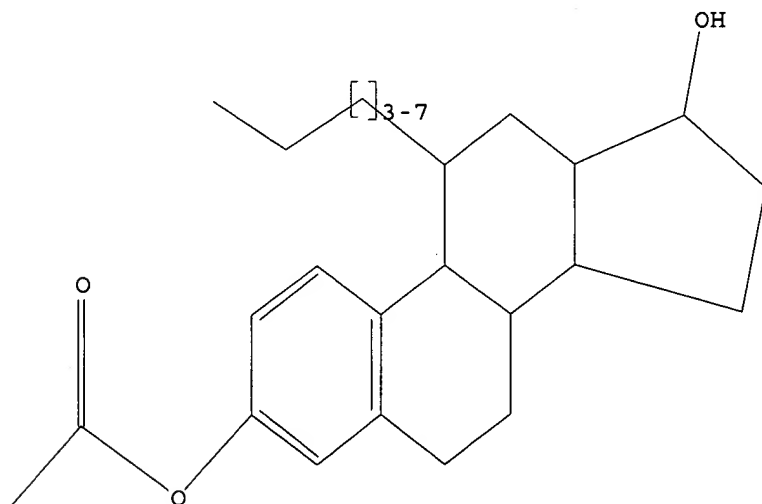
Uploading anna.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



steroids

09831954

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:22:08 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 23988 TO ITERATE

100.0% PROCESSED 23988 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L2 6 SEA SSS FUL L1

=> d 1-6

L2 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2002 ACS

RN 367269-94-1 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

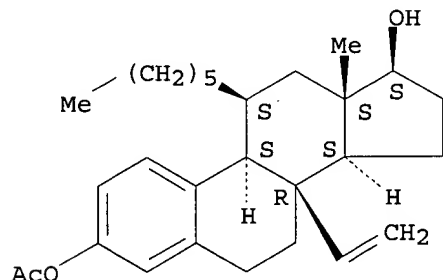
FS STEREOSEARCH

MF C28 H40 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2002 ACS

RN 367269-93-0 REGISTRY

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-hexyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

FS STEREOSEARCH

MF C28 H42 O3

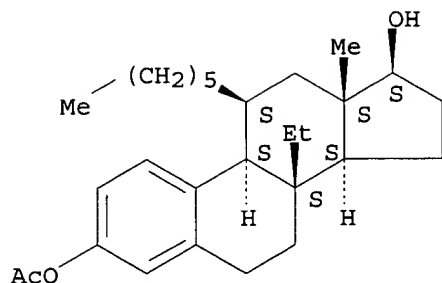
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

steroids

09831954

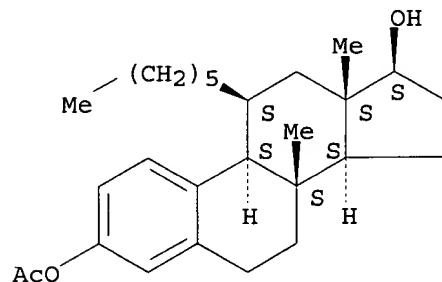


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2002 ACS  
RN 367269-92-9 REGISTRY  
CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate  
FS STEREOSEARCH  
MF C27 H40 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



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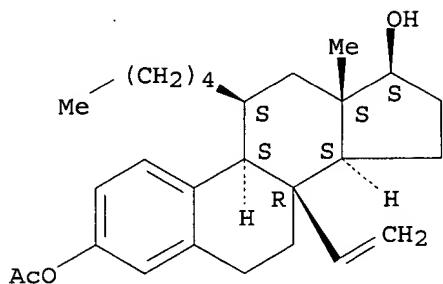
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2002 ACS  
RN 367269-91-8 REGISTRY  
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate  
FS STEREOSEARCH  
MF C27 H38 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

steroids

09831954

Absolute stereochemistry.

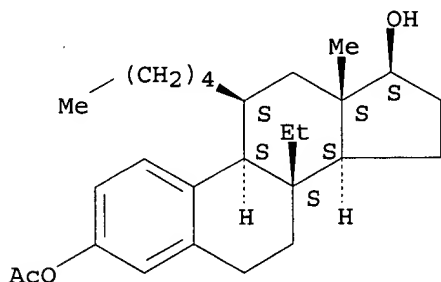


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L2 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2002 ACS  
RN 367269-90-7 REGISTRY  
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate  
FS STEREOSEARCH  
MF C27 H40 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

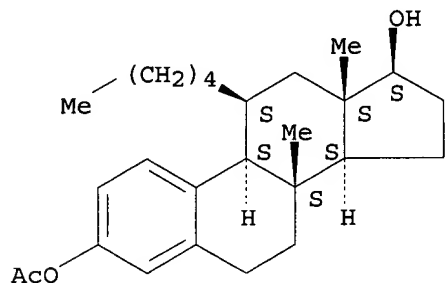
L2 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2002 ACS  
RN 367269-89-4 REGISTRY  
CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate  
FS STEREOSEARCH

steroids

09831954

MF C26 H38 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file ca caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
150.14	150.35

FULL ESTIMATED COST

FILE 'CA' ENTERED AT 14:22:31 ON 14 NOV 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE 'CAPLUS' ENTERED AT 14:22:31 ON 14 NOV 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

=> s l2  
L3 2 L2

=> d 1-2 .mano hitstr

L3 ANSWER 1 OF 2 CA COPYRIGHT 2002 ACS  
TI Preparation of 8.beta.-substituted-11.beta.-pentyl- and  
11.beta.-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity  
for the estrogen receptor  
SO PCT Int. Appl., 53 pp.  
CODEN: PIXXD2  
AB The present invention relates to the novel 8.beta.-substituted  
estra-1,3,5(10)-trienes I [R2 = H, F, Cl, Br, I, straight or branched  
(un)satd. C1-6-alkyl, OH, alkoxy, acyloxy, CF3, sulfamoyloxy; R3 = alkoxy,  
sulfamoyloxy, acyloxy; R6, R6' = H; R6R7 = bond; R7, R7' = H ; R8 means a  
straight-chain or branched-chain, optionally partially or entirely  
halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an  
ethynyl or prop-1-ynyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 =  
bond ; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy,

steroids

acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8.beta.-methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol (II) was prepd. from 8.beta.-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of estrogen receptor prepsns. of rat prostate than of estrogen receptor prepsns. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the prodn. thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

PY 2001

2001

IN Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2001077138 A1 20011018 WO 2001-EP4289 20010412

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

DE 10019167 A1 20011018 DE 2000-10019167 20000412

IT 367269-89-4P, 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-90-7P, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-91-8P, 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-92-9P, 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-93-0P, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-94-1P, 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of 8.beta.-substituted-11.beta.-pentyl- and -11.beta.-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the estrogen receptor)

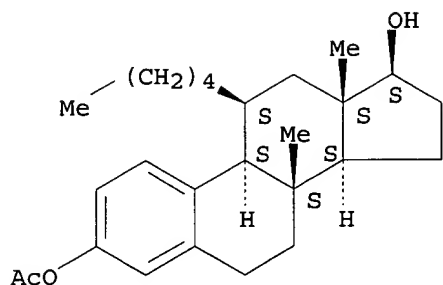
RN 367269-89-4 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

steroids

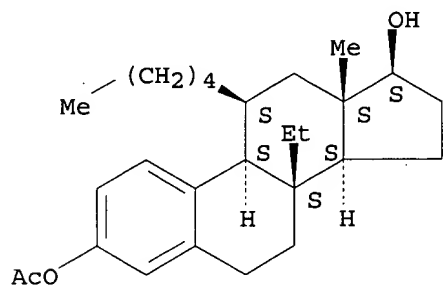
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RN 367269-90-7 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

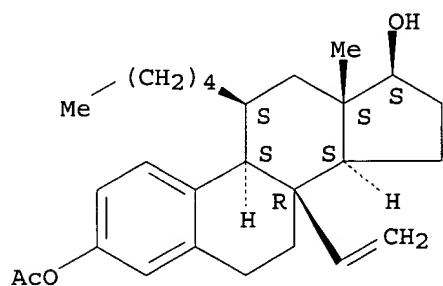
Absolute stereochemistry.



RN 367269-91-8 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



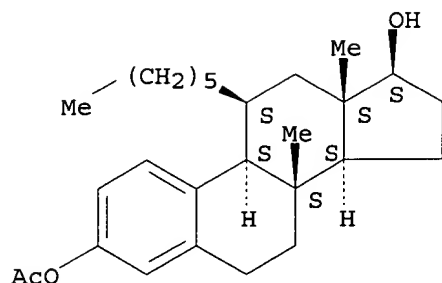
RN 367269-92-9 CA

CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

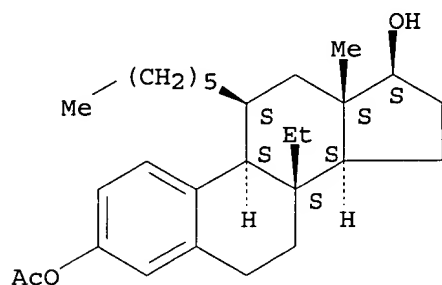
steroids

09831954



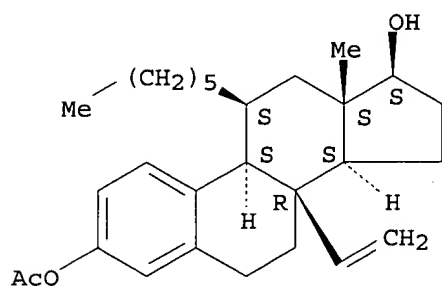
RN 367269-93-0 CA  
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-hexyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 367269-94-1 CA  
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-hexyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS  
TI Preparation of 8.beta.-substituted-11.beta.-pentyl- and  
11.beta.-hexyl-estra-1,3,5(10)-triene derivatives which have an affinity  
for the estrogen receptor  
SO PCT Int. Appl., 53 pp.  
CODEN: PIXXD2  
AB The present invention relates to the novel 8.beta.-substituted  
estra-1,3,5(10)-trienes I [R<sub>2</sub> = H, F, Cl, Br, I, straight or branched  
(un)satd. C1-6-alkyl, OH, alkoxy, acyloxy, CF<sub>3</sub>, sulfamoyloxy; R<sub>3</sub> = alkoxy,  
sulfamoyloxy, acyloxy; R<sub>6</sub>, R<sub>6</sub>' = H; R<sub>6</sub>R<sub>7</sub> = bond; R<sub>7</sub>, R<sub>7</sub>' = H ; R<sub>8</sub> means a

steroids



straight-chain or branched-chain, optionally partially or entirely halogenated alkyl or alkenyl radical having up to 5 carbon atoms, an ethynyl or prop-1-ynyl radical; R11 = pentyl, hexyl; R14 = H; R14R15 = bond; R15 = H; R15', R16' = H, F, Cl, Br, I, alkoxy, sulfamoyloxy, acyloxy; R15R16 = bond; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfamoyloxy; alkyl and acyl or acyloxy; alkoxy and alkyl, alkoxy and acyloxy; R17R17' = CH2 CR23R24; R23, R24 = H, halogen; R23R24 = O]. Thus, 8.beta.-methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol (II) was prepd. from 8.beta.-cyanosteroid III (R25 = CN) via condensation of 11-ketosteroid III (R25 = Me) with BuCH2Li. Estradienes I are used as pharmaceutical active agents which, in vitro, are provided with a higher affinity of estrogen receptor preps. of rat prostate than of estrogen receptor preps. of rat uterus and, in vivo, preferably act in a preferential contraceptive manner on the ovary without stimulating the uterus. The invention also relates to the prodn. thereof, the therapeutic use thereof and pharmaceutical administration forms which contain the novel compds. I. The invention further relates to the use of compds. I for male contraception and to the use of non-malignant or malignant proliferate diseases of the ovary, such as ovarian carcinoma or granulosa cell tumors for instance.

PY 2001

2001

IN Peters, Olaf; Braeuer, Nico; Hillisch, Alexander; Hegele-Hartung, Christa; Fritzemeier, Karl-Heinrich

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077138	A1	20011018	WO 2001-EP4289	20010412

PI

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

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DE 10019167 A1 20011018 DE 2000-10019167 20000412

IT

367269-89-4P, 8.beta.-Methyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-90-7P, 8.beta.-Ethyl-11.beta.-pentyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-91-8P, 11.beta.-Pentyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-92-9P, 11.beta.-Hexyl-8.beta.-methyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-93-0P, 8.beta.-Ethyl-11.beta.-hexyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate 367269-94-1P, 11.beta.-Hexyl-8.beta.-vinyl-1,3,5(10)-triene-3,17.beta.-diol 3-acetate

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 8.beta.-substituted-11.beta.-pentyl- and -11.beta.-hexyl-estra-1,3,5(10)-triene derivs. which have an affinity for the estrogen receptor)

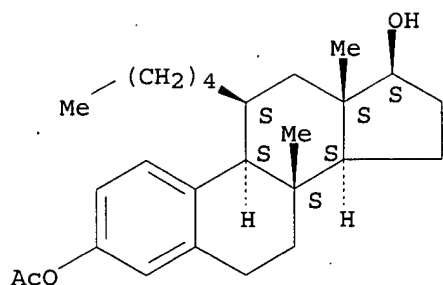
RN 367269-89-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-11-pentyl-, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

steroids

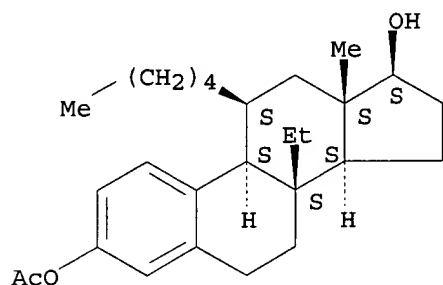
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RN 367269-90-7 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

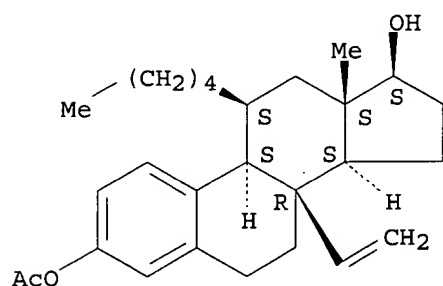
Absolute stereochemistry.



RN 367269-91-8 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-11-pentyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



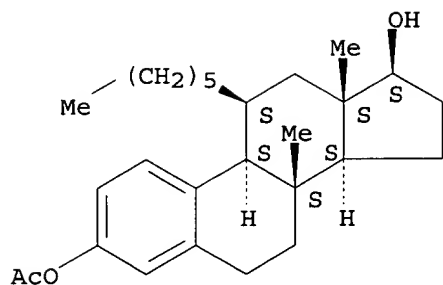
RN 367269-92-9 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 11-hexyl-8-methyl-, 3-acetate,  
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

steroids

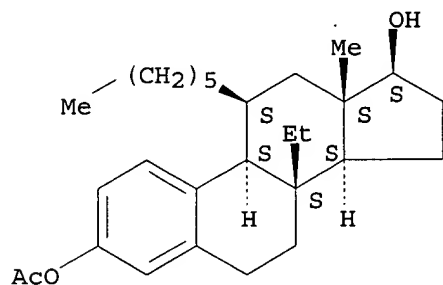
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RN 367269-93-0 CAPLUS

CN Estradiol, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

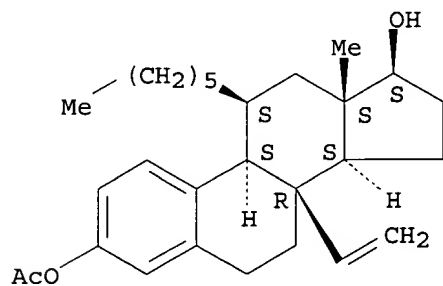
Absolute stereochemistry.



RN 367269-94-1 CAPLUS

CN Estradiol, 3-acetate, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=>

steroids